Modeling Urea-Based SNCR in a Gas-Fired Utility Boiler

Eric G. Eddings, Jacob Brouwer and Michael P. Heap

Reaction Engineering International

Salt Lake City, Utah

Felix E. Spokoyny

Wahlco, Inc.

Santa Ana, California

A retrofit operation is underway whereby urea-based SNCR is being installed on four identical opposed-wall gas-fired boilers at Permenergo's Tchaikovsky Plant located near Perm, Russia. Access to optimal regions for SNCR reagent injection is limited; therefore, computational-fluid-dynamics (CFD) modeling for reacting, two-phase flows was utilized to assist in locating injectors and evaluating reagent mixing and NOx reduction.

To address this type of problem, a three dimensional CFD-based turbulent reacting flow model was modified to include:

- Tracking of urea/H2O droplet cloud trajectories within the computational domain, with subsequent water evaporation, drying, and urea decomposition to gas-phase products.
- Chemical kinetic mechanism for the prediction of selective non-catalytic reduction (SNCR) chemistry.

The second issue was particularly challenging, and a reduced mechanism for gas-phase SNCR chemistry developed by REI was utilized to quantify the levels of NOx reduction in the gas phase. The reduced mechanism (7 reactions) and individual rate constants were developed so that the mechanism could be incorporated into a CFD code (Brouwer et al., 1996). The model accurately describes the SNCR chemistry as indicated by comparison of NOx reduction efficiency, ammonia slip and N2O emissions with predictions obtained using a complete chemical mechanism (296 reactions) and experimental measurements from independent investigators.

The SNCR submodel was incorporated into GLACIER, a computer code, which places particular emphasis on the simulation of combustion phenomena and pollutant formation in either gaseous, liquid or solid fuel combustion. The combustion simulation tool, GLACIER, solves the governing gaseous fluid mechanics and reaction equations in an Eulerian framework. The gas phase is assumed to be a turbulent, reacting continuum field that can be described locally by general conservation equations. Gas properties (i.e., density, temperature, species composition) are determined through local mixing calculations, and are assumed to fluctuate randomly according to a probability density function (PDF) which is characteristic of the turbulence.

The effects of particle or droplet-phase mechanics and multiphase reactions are calculated in a Lagrangian frame of reference. Particle mass and momentum sources are converted from a Lagrangian to an Eulerian reference frame where they are coupled with the gas phase fluid mechanics. The dispersion of the particle or droplet cloud is based on statistics gathered from the turbulent flow field, and heat, mass, and momentum transport effects are also included for each cloud. The radiative heat transfer is

computed using the discrete ordinates method and is fully coupled with the turbulence.

Simulation of these boilers required great computational resolution around the gas burners in the lower furnace and around the relatively small diameter urea solution injectors in the upper furnace. To allow for the necessary mesh resolution in both the upper and lower furnace regions and also to maintain an acceptable turnaround time for the computer simulations, the problem was divided into two halves: the lower furnace and the upper furnace.

Lower furnace combustion simulations were performed of Units 1 & 2, firing natural gas at full and reduced loads. Temperature measurements were available for the two units at reduced load conditions and these measurements were utilized to calibrate unknown thermal boundary conditions (outlet and wall emissivities) in the simulations while operating at lower loads. Using the calibrated boundary conditions, simulations were then performed for both boilers operating at full load (420 tph) to provide information necessary for design of a urea injection system in the upper furnace.

To evaluate various designs of the upper furnace injection system, simulations were performed of the upper furnace regions of Unit 1, and the information from the lower furnace simulation was mapped onto the inlet of the upper furnace model. Different injection configurations were simulated to determine mixing effectiveness of the injection design, as well as overall NOx reduction efficiency.

The baseline case utilized injection from the front wall only at the highest possible elevation for injection (3/4 of the way between the furnace nose and the boiler roof). Temperature conditions were appropriate for SNCR reactions but flow coverage with reagent was inadequate. The analyses allowed identification of a strong vortical bag close to the injection area. This recirculation zone had drastically different effects on the trajectories of injected droplets depending on size distribution and aiming angles. NOx reduction within this circulation pattern was extremely high but the main body of the flue gas stream was flowing around this zone.

In order to increase the flow coverage, some reagent was introduced at a lower level (1/3 of the way between the furnace nose and the boiler roof). Calculations indicated significant amounts of oxidation of the SNCR reagent, thus resulting in lower overall net reduction.

To improve reagent distribution in zones close to the side walls, additional injectors were included on the side walls near the furnace nose. The results indicated that measurable amounts of the urea solution exited the simulation without completely evaporating and entering the gas phase. Later, the side wall injectors were moved more towards the front wall of the furnace to avoid impinging on the shield tubes and improve chemical utilization.

Simultaneous analyses of distributions of the gas flow, ammonia and NOx concentrations in the domain outlet cross section, allows identification of more or less efficient injector locations. The best injection pattern determined in the computer simulations is used as a starting point for field optimization.

Thus, given the constraint of a limited number of access ports in the upper furnace, the CFD tool was able to assist in the identification of an optimized reagent distribution, relative level of NOx reduction, and extent of ammonia slip by evaluating various injector locations and patterns prior to performing more costly field trials.

References

Brouwer, J., Heap, M.P., Pershing, D.W., and Smith, P.J., 1996, "A Model for Prediction of Selective Noncatalytic Reduction of Nitrogen Oxides by Ammonia, Urea and Cyanuric Acid with Mixing Limitations in the Presence of CO," Twenty-Sixth Symposium (International) on Combustion, The Combustion Institute, *in press*.